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Electron Transport in Si Nanowires

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Abstract. We investigate electron transport in silicon nanowires taking into account acoustic, non-polar optical phonons and surface/interface roughness scattering. We find that at very high transverse fields the reduced density of final states to which the carriers can scatter into gives rise to a reduced influence of interface-roughness scattering, which is promising result from a fabrication point of view.

1. Motivation and Model Description

Nanowires (NW) and nanotubes are expected to exhibit one-dimensional (1D) transport and hence improved mobility due to the reduced density of states for scattering [1] and reduced number of propagating modes. The enhancement of phonon limited mobility due to subband modulation in ultrathin SOI MOSFETs has also been reported [2]. Although there have been claims of high electron mobility in silicon nanowires [3,4], recent paper [5] contradicts these results. Kotlyar, *et al*., investigated the phonon limited mobility in a cylindrical SiNW and found it to be no better than the one in two-dimensional (2D) MOSFETs. The objective of this paper is to investigate the mobility of electrons in a rectangular SiNW, by taking into account the major scattering mechanisms such as acoustic phonon, non-polar optical phonon, and surface roughness scattering. The effect of surface roughness is considered using two different models. The phonons are treated in bulk mode approximation. The effect of the phonon confinement is not taken into consideration in calculating the scattering rates. The modification of the phonon spectrum due to spatial confinement [6] is expected to enhance the overlap of the electron and confined phonon wave function, thus increasing the electron-phonon scattering. This increase is not expected to be significant [5] for the dimensions considered in this work. The paper is organized as follows: Section 2 describes the various components of the simulator used in the mobility calculation. The device structures used in this study and the corresponding simulation results are presented in Section 3. We finish this work (Section 4) with some conclusive remarks regarding the research done and directions for future research.

2. Simulator Components Description

The device considered for this research work is described in more details in Ref. [7]. Briefly, the SOI device structure consists of a 100 nm silicon substrate, on top of which is grown 80 nm of buried oxide. The thickness of the SOI layer is 8 nm and the width is 30 nm (varies to 8 nm). On top of the SOI layer sits the gate-oxide layer with thickness of 25 nm. This device has been used to compare the mobility data obtained by Takagi *et al*. [7] for a 2-d electron gas. The doping in the channel is 3×10^{15} cm^{-3}.

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Note that the silicon nanowires considered in this study have spatial confinement along the *x* and the *y* direction. The electrons are free to move only in the *z* direction. To obtain any macroscopic quantity of interest such as mobility, we need to follow two steps: (1) Solve the Poisson and Schrödinger equations self-consistently, (2) Solve the Boltzmann Transport Equation (BTE) using the Monte Carlo method (use the results from (1)). In the rest of this section, we briefly describe these two solvers.

2.1. 3D Poisson-2D Schrödinger Solver

We begin by setting up the structure file and defining the grid for solving the discretized Poisson equation. To calculate the electron density in the confined directions, we solve the discretized Schrödinger equation in the SOI layer. The wave function penetration is taken into account by including few mesh points in the oxide region. Setting up the mesh forms the initialization process. Then the discretization coefficients are calculated and the Poisson equation is solved using Incomplete LU decomposition method (ILU) [8]. The central coefficient that results from the discretization of Schrödinger equation is then calculated using the potential obtained from the Poisson solver and the Schrödinger equation is solved for the required number of subbands. In the next iteration loop, the electron density *n* in the channel is calculated. The charge density is updated with this *n*. This procedure is continued until the potential convergence criterion is reached. Then, the required data, potential profile, wavefunctions and the subband details are written into files. These are then used in the Monte Carlo method described in Section 2.2 below. Sample simulation results for the confinement along the depth and width of the device are shown in Fig. 1.

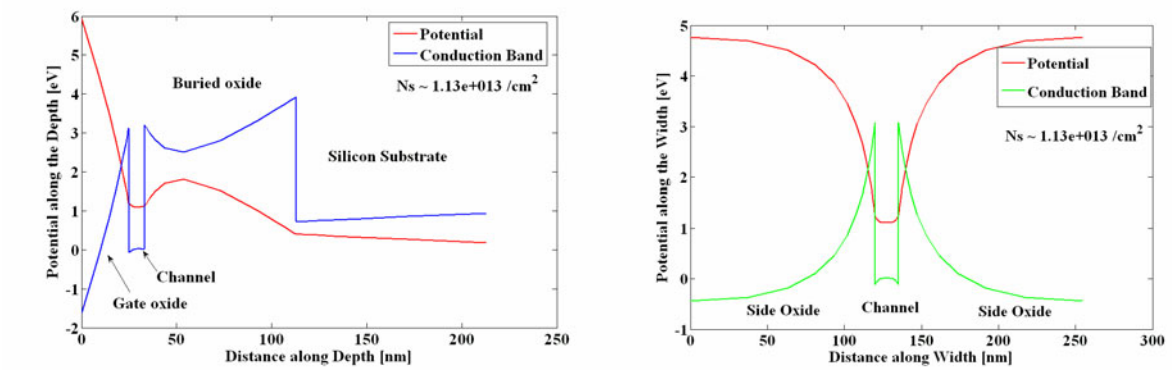

Figure 1. Confining potential profile along the depth (left panel) and width (right panel) of the wire.

2.2 1D Monte Carlo Transport Kernel

The Monte Carlo transport kernel is the standard one except for the fact that when we calculate the scattering rates for various scattering mechanisms included in the model (acoustic phonons, intervaley non-polar optical phonons and interface-roughness scattering) an additional complication is to calculate the various overlap integrals that appear in the final expressions. In all our simulations we have used non-parabolic band model. The scattering rates for acoustic, intervalley and surface-roughness scattering are shown in Fig. 2.

3. Simulation Mobility Results

The simulator developed is verified by plotting the mobility of a wire of width 30 nm and comparing it with the mobility obtained for 2-d electron gas in the experiment presented in Ref. [7]. The results shown in Figure 3 exhibit very good agreement with the experimental data. Note that electrons in a wire of width 30 nm can be assumed to behave just like those in a 2-d gas, because the confinement along the width is very low. We see that the simulation data overestimate the mobility at mid transverse electric fields. This is attributed to the fact that confined phonons, which are not taken into account in this study, will lower the mobility values in the region where phonons dominate transport,

which is the mid-effective field region. Having verified the simulator the next thing to do is to estimate the mobility behavior with decreasing the wire width. The results presented in Figure 4 show the variation of mobility with effective field for wires of width 30nm, 15nm and 8nm.

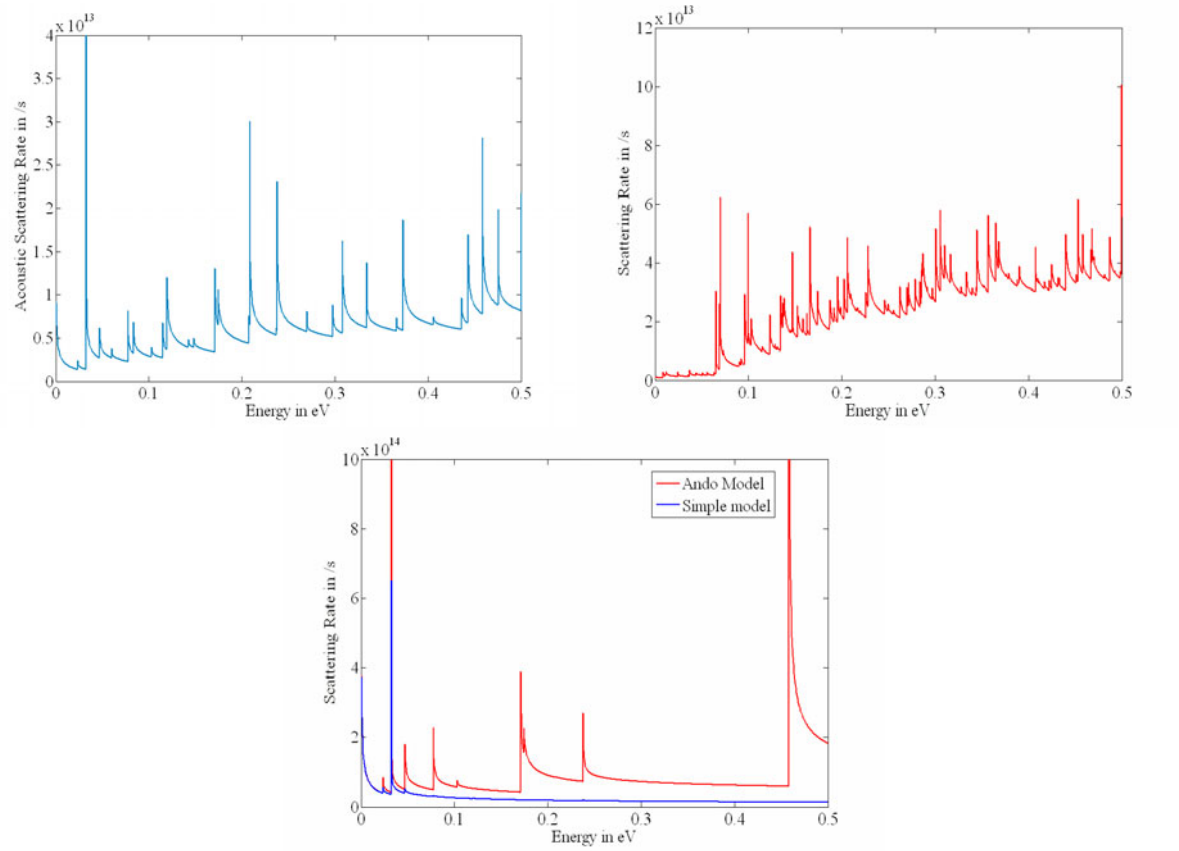

Fig. 2 Acoustic phonon scattering rate as a function of energy for a 10nm wire for sheet density $N_s \sim 10^{13}/cm^2$ (top left panel); Non-polar optical phonon scattering rate as a function of energy for a 10nm wire for sheet density $N_s \sim 10^{13}/cm^2$ (top right panel); Surface Roughness scattering rate as a function of energy for the two models considered (10nm wire for sheet density $N_s \sim 10^{13}/cm^2$).

4. Conclusions

Self-consistent 3-d Poisson 2-d Schrödinger solver was developed and the potential and wavefunctions from it were fed into the 1-d Monte Carlo simulator to solve the BTE and study the mobility of electrons in a rectangular silicon nanowire transistor. To test the simulator, first the mobility of electrons in a 30 nm wide wire (wherein the electrons behave as though they are confined only along the thickness), was matched with the experimental mobility obtained for a 2-d electron gas with same SOI thickness. Then the effect of decreasing width on the mobility of electron was studied.

Acoustic phonons, non-polar optical phonons and surface roughness scattering were included in the Monte Carlo kernel to model the transport of electrons. The effect of phonon and roughness scattering, together and individually, on the mobility of electrons were analyzed for various widths of the nanowire. Surface roughness scattering was modeled using two approaches and it was found that the usual method adopted for modeling the surface roughness underestimates the scattering rate. Ando's model [9] is found to give much better result.

Surface roughness scattering is found to decrease with decreasing width, for widths in the range between 30 nm and 8 nm, since the electrons prefer the side channel to the top channel, as the width

decreases. This results in an enhanced mobility. Phonon limited mobility is found to decrease with decreasing width, and this is attributed to the increase of electron wavefunction overlap. This increase in overlap is expected to be more pronounced if the effect of confined phonons is included.

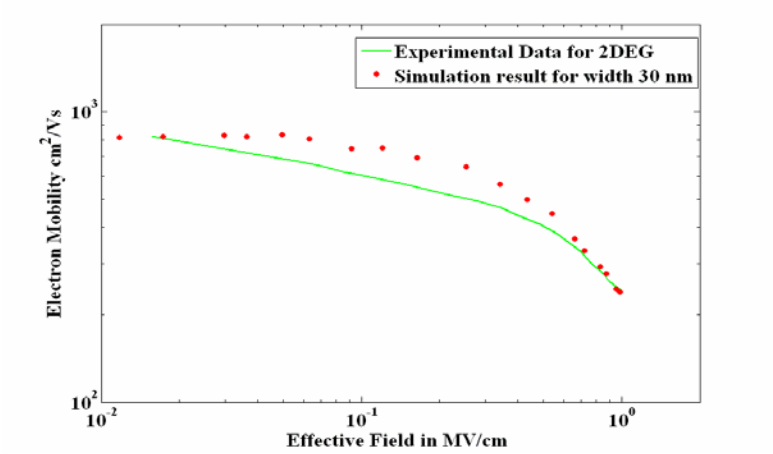

Figure 3. Electron mobility of a 30nm wide wire and 2-d electron gas.

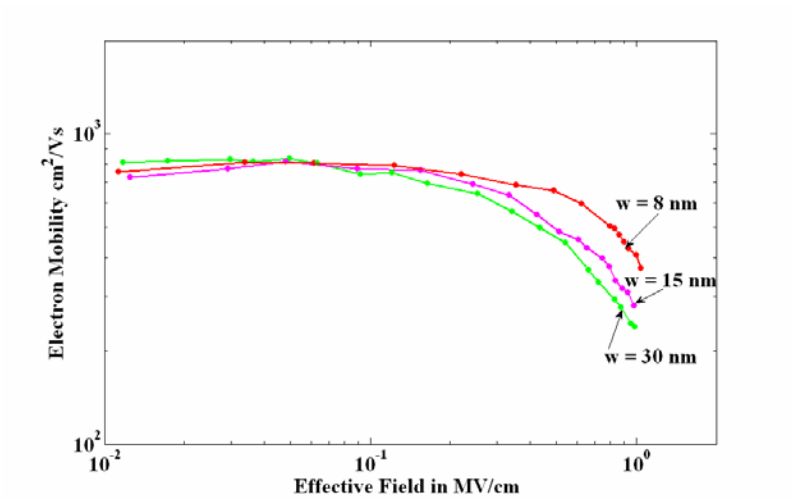

Figure 4. The variation of electron mobility with the width of the nanowire.

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